

Product Information

Renin-angiotensin-aldosterone system (RAAS) inhibitor, Obeticholic acid, Purity $\geq 98\%$

Cat. No.: X24-09-YM309

Size: 10 mg; 20 mg; 50 mg; 100 mg

CAS Number: 459789-99-2

Compound CID: 447715

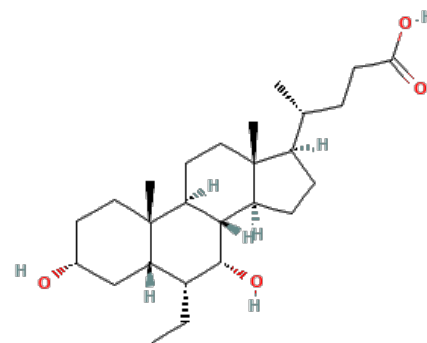
Synonym: 459789-99-2; INT-747; 6-ECDCA;

(4*R*)-4-[(3*R*,5*S*,6*R*,7*R*,8*S*,9*S*,10*S*,13*R*,14*S*,17*R*

)-6-Ethyl-3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahy

dro-1*H*-cyclopenta[*a*]phenanthren-17-yl]pentanoic acid; Renin-angiotensin-

aldosterone system (RAAS) inhibitor



This product is for research use only and is not intended for diagnostic use.

Product Information

Description	Obeticholic acid, soluble in DMSO and ethanol and insoluble in water, is an effective metabolism inhibitor, that has the ability to prevent the pathway of cell metabolism by inhibiting FXR. The molecular weight of the compound is 420.63, and its molecular formula is C ₂₆ H ₄₄ O ₄ . It targets the FXR.
Molecular Weight	420.63
Molecular Formula	C ₂₆ H ₄₄ O ₄
Targets	FXR
IUPAC Name	(4 <i>R</i>)-4-[(3 <i>R</i> ,5 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,8 <i>S</i> ,9 <i>S</i> ,10 <i>S</i> ,13 <i>R</i> ,14 <i>S</i> ,17 <i>R</i>)-6-Ethyl-3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1 <i>H</i> -cyclopenta[<i>a</i>]phenanthren-17-yl]pentanoic acid
InChI	InChI=1S/C26H44O4/c1-5-17-21-14-16(27)10-12-26(21,4)20-11-13-25(3)18(15(2)6-9-22(28)29)7-8-19(25)23(20)24(17)30/h15-21,23-24,27,30H,5-14H2,1-4H3,(H,28,29)/t15-,16-,17-,18-,19+,20+,21+,23+,24-,25-,26-/m1/s1
InChI Key	ZXERDUOLZKYMJM-ZWECCWDJSA-N
Canonical SMILES	CCC1C2CC(CCC2(C3CCC4(C(C3C1O)CCC4C(C)CCC(=O)O)C)C)O
Form	Lyophilized powder



Purity	≥98%
Impurities	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
Solubility	<i>In vitro</i> : DMSO: 76 mg/mL (180.68 mM); Water: insoluble; Ethanol (warmed): 76 mg/mL (179.76 mM)
Identity	Confirmed by NMR/HPLC/MS.
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	Obeticholic acid can be used for its protective effects against metabolic diseases.
Storage	Store at -20°C, and keep desiccated.
